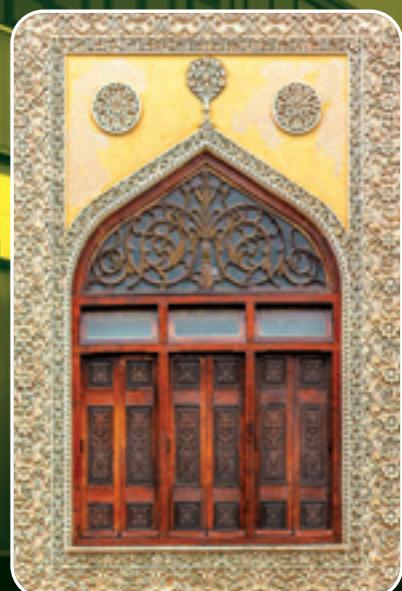


Crystallography News

British Crystallographic Association

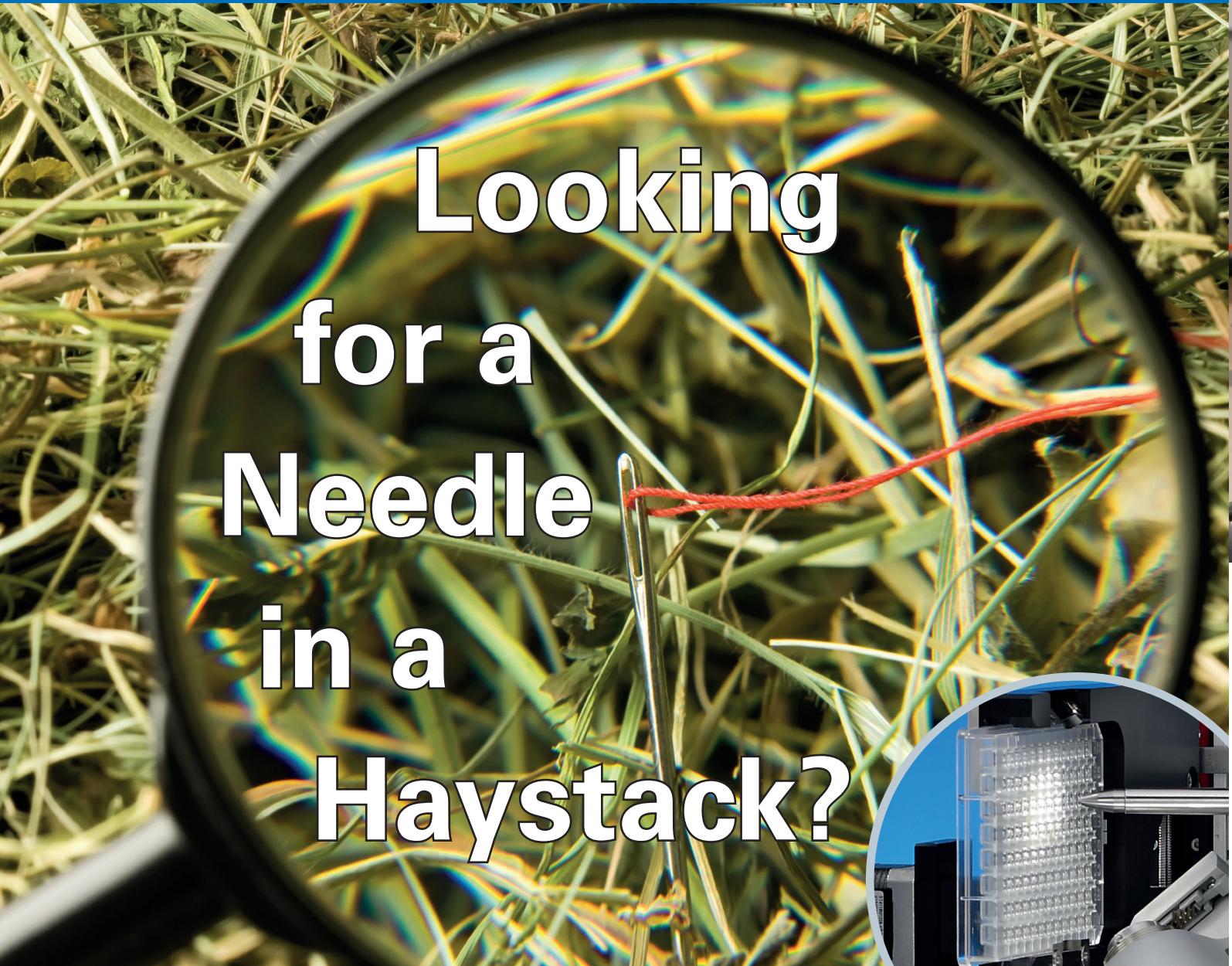
Issue No. 140 March 2017

ISSI 1467-2790



Lancaster and Hyderabad await; Dschang succeeds

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Easier Access to Data Deposited with CCDC	p22



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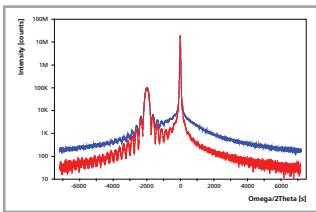
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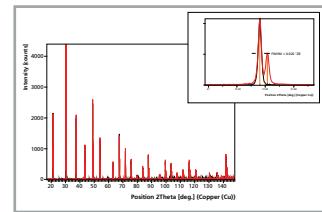
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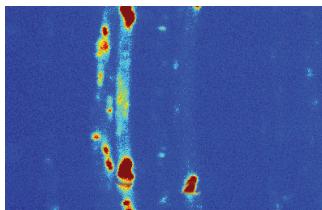
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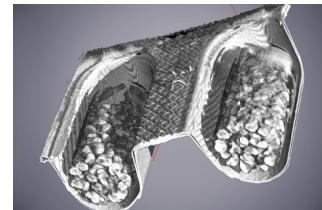
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2D



3D



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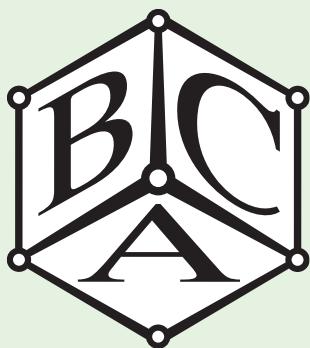
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Crystallography News March 2017

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Cover photographs of India:
Charminar, courtesy of Gopikrishna Narla.
Palace window, courtesy of Rohit Sarma.

This month's cover:

Lancaster exhibition venue
and city view, Hyderabad
landmarks, Pan-African
Conference scenes



From the President



I HAVE found myself reflecting recently, as have many in the scientific community, on the importance of international friendship and collaboration in science. With the current uncertainties in international politics, it is important that we maintain strong links with scientists around the world and oppose

initiatives that weaken such links. I can speak personally of the benefits of having lived and worked overseas, travelled to many countries because of science, collaborated with scientists from other countries, worked with colleagues and students from other countries and simply found friendships with scientists from around the world. Long may such opportunities continue – to the benefit of science and human development. In the crystallographic community we are in the year of our triennial international cycle in which the IUCr Congress is held. This August the Congress will be held in Hyderabad, its first visit to India, a country with a thriving crystallographic community. I hope many from the UK will take the opportunity to attend and participate in the meeting. Last year marked the First Pan African Conference of Crystallography held in Dschang (Cameroon), 6-10th October, 2016. It was a great success and included 205 participants of 32 nationalities. The BCA contributed some funds to provide bursaries for students studying in Africa to attend the conference. It is expected that the conference will lead to the foundation of AfCA, the Africa Crystallography Association. A steering committee led by Prof. André Roodt (University of the Free State, Bloemfontein, South Africa) is currently developing this initiative. There are plans for a second conference in 2018.

Closer to home, I am looking forward to the upcoming BCA Spring Meeting in Lancaster. At the time of writing this column, the abstract deadline has recently passed, and there is an excellent line-up of symposia, speakers and poster presenters. Lancaster also offers the opportunity to combine the meeting with a visit to the Lake District, which I'm sure some attendees will take advantage of. I am grateful to Programme Chair Andrew Bond and the whole Programme Committee for their commitment over the past year in putting the meeting programme together, and to our colleagues at Hg3 for again smoothly handling the logistical side of the conference planning and delivery. The main meeting will feature Awards lectures from Kay Diederichs, who will give the Lonsdale Lecture, and Mike Glazer, who will give the Bragg Lecture. Wednesday afternoon will include the Early Career Awards Symposium, featuring lectures from the awardees of the BCA groups. The Annual General Meeting will be held during its usual Wednesday early evening slot and will see elections for the positions of Treasurer and one of the three Ordinary Member positions on Council. There will also be discussion and voting on a proposal being put forward by Council to make changes to the way in which Council members are nominated and voted for. This proposal will be formulated based on Council discussions that have already taken place and the informal consultation with the membership which is underway. Prior to the BCA AGM the AGMs for the

BSG, CCG, IG and PCG groups will be held (earlier that day) and will include committee member elections (AGM for the YCG is on the Monday). I'd like to take this opportunity to encourage members to stand for committee positions of the groups. The groups are the foundation of the BCA and have a vital role in enabling the Spring and Winter meetings to provide a forum for discussion of structural science in all its breadth.

As we await the outcome of applications for the new BCA-funded Education and Outreach Programme to develop resources that can be used by schools and the crystallographic community at large, I'd like to highlight an excellent crystallographic outreach project that has been developed at Diamond Light Source. Known as **Project M** – 1000 samples, 100 schools, one great big experiment – the project has allowed schools to enrol and receive a kit from which they can grow crystals of calcium carbonate in the presence of 10 different additives. The 1000 samples generated by the 100 participating schools will be analysed by PXRD in one 24-hour period at Diamond beamline I11 – no mean feat in itself! The project will evaluate which of the three polymorphs, vaterite, calcite or aragonite form under each of the conditions. The project has been developed by **Claire Murray, Julia Parker and Laura Holland** at Diamond together with **Rebecca O'Brien** at the Wellcome Trust.

The project was officially launched on Dec 5th with some help from Prof. **Alice Roberts**.

You can find out more at <http://www.diamond.ac.uk/ProjectM/>. I await the results with great interest. Discussion of crystals in schools also gives me an excuse to show a tremendous picture of a crystal grown as part of an IYCr schools competition in Croatia in 2014-15, which was sent to me recently by Prof. **Stanko Popović** (University of Zagreb).

Picture by K. Molcanov



I will close the column with the sad news of the recent death of Prof. **Howard Flack** (University of Geneva) on February 3rd, aged 73. Howard was internationally well known in the crystallographic community and made major contributions to the field over a number of years, but will always be associated with his contributions to understanding absolute configuration and what became known as the Flack parameter. I met Howard a number of times over the years at conferences around the world – he was always someone I enjoyed talking with. He will be sadly missed.

Lee Brammer



BCA Council 2017

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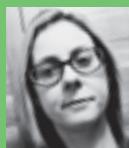
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Full committee details on the
BCA website

www.crystallography.org.uk

From the Editor



OUR Groups have all held their Autumn or Winter Meetings. The reports in this issue show that the standard of the presentations was world-class. For instance, the BSG Winter Meeting started off with a lecture by Sir Tom Blundell. He has been awarded the great honour of the Ewald Prize, the presentation of which will open the scientific

proceedings at the Congress of the International Union of Crystallography that will take place in Hyderabad this coming summer – but you heard him speak to the BSG first!

On the subject of Hyderabad, I am delighted to publish a letter of invitation from **Gautam Desiraju**. Along with holding a glittering array of appointments (Immediate Past President of the IUCr, and Chairman of the Local Organizing Committee and the International Program Committee for the 24th IUCr Congress), Gautam has long been a good friend of the BCA. Gautam's letter describes the exciting programme and the effort made to ensure comfort and convenience for participants. Let me remind you to study the conference website carefully. When going to international conferences, we are accustomed to showing our passports to the immigration officers and getting waved straight through. India is different. Foreigners entering India need to obtain an entry visa. Getting a visa is not a problem; but as with any bureaucratic endeavour, it takes time, on the order of 2 months. There is a distinction between tourist visas and conference visas. Attending the Congress of the IUCr requires a conference visa, which also allows tourism. On the other hand, a tourist visa would not allow participation in the Congress. Two important deadlines should be kept in mind: bursary applications close on 15 March and Early Bird registration closes on 31 May.

Of course, we'll have an exciting meeting earlier than that: our own BCA Spring Meeting in Lancaster from 10-13 April. One of our cover pictures shows the LICA building, which will be the venue for the exhibition, posters and meal and tea breaks. It has a water feature which looks as if it should be attractive to ducks – and BCA meetings are always better with ducks! Up-to-date details appear in this issue. If you act quickly, you are still in time to take advantage of Early Bird registration, which will close on 10 March. We also introduce **Lauren Hatcher**, this year's winner of the CCG Prize which will be awarded at this meeting.

Our Industrial Group has a snazzy new logo, and a new and improved website will follow shortly; but one tradition remains the same: the holding of an XRF/XRD meeting in June at the University of Leicester. This year the date will be the 14th of June for the XRF section and the 15th for XRD. See the IG website for programme updates. The annual autumn IG meeting will take place in November 2017, the date and venue to be confirmed.

With the meeting of the German Crystallographic Society starting on 27 March this year, a couple of weeks later than in

previous years, there is still time to arrange your attendance. The great strength of Germany in the crystallography of materials is reflected in these meetings. Other topics in a wide-ranging programme are displayed on the website, <http://www.dgk-conference.de/>. The official language is English. An additional incentive is the location of the conference in Karlsruhe, Baden, not far from the Black Forest. Baden is across the Rhine from France, and its inhabitants are said by other Germans to share some of the French *joie de vivre* and love of wine.

Aficionados of jazz and the “resolution revolution” can enjoy the meeting of the American Crystallographic Association in New Orleans this May. The first plenary lecture will be given by 2016 Nobel Laureate in Chemistry, Sir **James Fraser Stoddart**, and the topic of this year's Transactions Symposium is “Going Beyond PX with Cryo Electron Microscopy, Tomography, and Diffraction”. The deadline for submission of abstracts was 15 February, but a sufficiently interesting abstract and a persuasive appeal to the Special Relationship might still get you a poster presentation. The Early Bird registration deadline is 31 March.

We are very fortunate that crystallographic databases provide easy access to a wealth of accumulated data. In addition, the Cambridge Crystallographic Data Centre and International Centre for Diffraction Data have been loyal supporters of the BCA. In this issue we have an article about the enhanced procedure for accessing one's structures deposited with the CCDC. The CCDC also supported the First Pan-African Conference on Crystallography, and people affiliated to CCDC have contributed the reports here. The ICDD has some important news, too: the appointment of a new Executive Director, **Tom Blanton**. A profile of Tom outlining his background and his previous work for ICDD can be accessed by clicking on the News column on the ICDD website.

I think that our “Meetings of interest” section is particularly rich in interesting and useful courses and schools. I mention three of them here, for which I have specifically been sent information. The ICDD will run several training courses on X-ray fluorescence and X-ray powder diffraction at their headquarters in Newtown Square, Pennsylvania. Oak Ridge National Laboratory offers a workshop on neutron scattering applications in structural biology in the beautiful foothills of the Appalachian Mountains. International applicants are welcome; but in view of the limited number of places they will need to make a good case. In a different area of structural science but in particularly beautiful surroundings, the second summer school on Total Scattering for Nanotechnology will take place at Lake Como. Again places are limited; an early application is advisable.

If this column gives the impression of being one of those tourism brochures that appear in the winter and early spring each year, I can cite as justification the decision by the UN to designate 2017 as the International Year of Sustainable Tourism for Development. I hope that each of you will find somewhere enjoyable to visit during this spring and summer, and your footprints will be light.

Carl Schwalbe

BCA Corporate Membership



The BCA values its close ties with commercial companies involved with crystallography. To enhance these contacts, the BCA offers Corporate Membership. Corporate Membership is available on an annual basis and includes the following benefits:

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Puzzle Corner



EACH of the three sets of clues will point you to the 9-letter name of a different element. The numbers from 1 to 9 correspond to letters. Different numbers could match the same letter. Deduce the correspondence for the words represented by the clues and enter the letters into the grid.

Clues for Element 1:

- 12945 is the name of a girl (who likes crystals?)
3512 is intense anger
867 is short for an institution of higher learning

1	2	3	4	5	6	7	8	9

Clues for Element 2:

- 234789 is the genus of plants including onion and garlic
13276 is Scottish fabric or a Welsh party
4591 is a light source

1	2	3	4	5	6	7	8	9

Clues for Element 3:

- 2453 is a house used for drying hops
6891 is a drainage receptacle
49765 is not quite right

1	2	3	4	5	6	7	8	9

Answer to December Puzzle Corner on page 10

Crystallography News March 2017

BCA Spring Meeting

University of Lancaster, 10-13 April 2017



BCA 2017

From the BCA 2017 Programme Committee

AT the time of writing this message, the scientific programme for the BCA Spring Meeting is close to complete. The named lectures promise to be outstanding and there is an exciting mix of sessions that we hope will appeal to the broad scientific interests of the BCA membership. Updates and further details will continue to be posted on the meeting website:

<http://bcaspringmeetings.org.uk>. Online registration remains available until Tuesday 4th April 2017. We are looking forward to seeing you in Lancaster.

Andrew Bond
Programme Committee Chair

The 2017 BCA Named Lecturers are:

Bragg Lecture

Prof. **Mike Glazer** (University of Oxford)
The wondrous world of perovskites

Lonsdale Lecture

Prof. **Kay Diederichs** (Universität Konstanz)
Towards a better understanding of (non-)isomorphism in macromolecular crystallography

The Plenary speakers are:

BSG: **James Naismith** (University of St. Andrews)
The structural biology of natural product biosynthesis

CCG: **Santiago Alvarez** (Universitat de Barcelona)
Transition metal coordination polyhedra: shape, spin and secondary bonding

IG: **David Rugg** (Rolls Royce)
Crystallurgy for aerospace and nuclear sectors: an industrial perspective of the next decade

PCG: **Sharon Ashbrook** (University of St. Andrews)
Investigating disorder and dynamics in solids using NMR spectroscopy

Scientific Programme

Monday 10 April (13:30) – Tuesday 11 April (11:15)

Young Crystallographers Group (YCG) Meeting

Plenary speakers:
Stefan Kaskel (Technische Universität Dresden)
Simon Coles (University of Southampton)

Teaching session: *How the other half live*

Keynote speakers:
Matthias Gutmann (ISIS)
Helen Playford (ISIS)
Jane Endicott (University of Newcastle)

Main Meeting

Tuesday 11 April, 2017

11:30 – 12:15

Lonsdale Lecture

Prof. **Kay Diederichs** (Universität Konstanz)
Towards a better understanding of (non-)isomorphism in macromolecular crystallography

13:30 – 14:15

CCG Plenary

Santiago Alvarez (Universitat de Barcelona)
Transition metal coordination polyhedra: shape, spin and secondary bonding

14:20 – 15:50

Extreme Conditions (PCG)

Chair: **Alex Gibbs** (ISIS)

Working at extreme conditions can often provide critical access to particular areas of phase space and therefore deep insight into the behaviour of materials, along with surprises not predicted by current theory. The session will cover scientific and technological developments across a wide range of extreme experimental conditions such as high magnetic field, high temperature, low temperature and high pressure.

Keynote: **Stephen Blundell** (University of Oxford)
Muon-spin rotation in extreme conditions

Lucy Clark (University of Liverpool)
Low-temperature spin liquid behaviour in the triangular-honeycomb XY antiferromagnet, $TbInO_3$

Göran Nilssen (ISIS)
My misadventures with magnets: spin waves in square lattice compounds

Hamish Yeung (University of Oxford)

When anomalous mechanics are hidden: a supramolecular mechanism for negative linear compressibility

14:20 – 15:50

Computational Approaches (CCG)

Chairs: Anthony Reilly (CCDC), Krešo Bučar (UCL)

The session will highlight computational methods in crystallography, crystal chemistry, materials science and crystal engineering. Emphasis will be on computational approaches aiding crystal-structure prediction and elucidation, structure-property correlations and predictions of physicochemical properties of organic, metal-organic and inorganic materials.

Keynote: **Colin Seaton** (University of Bradford)

Replicate, divide, mutate, survive: applying differential evolution optimisation to crystals

Doris Braun (Universität Innsbruck)

Exploring the crystal form landscapes of the alkaloids brucine and strychnine

Andrew Maloney (CCDC)

Structural properties from structural formulae: what can we learn from solid form landscapes?

Wojciech Ślawinski (ISIS)

Layered double hydroxides: how can we model structural disorder by X-ray powder diffraction?

14:20 – 15:50

Anti-Microbial Targets (BSG)

Chair: Lydia Tabernero (University of Manchester)

Infectious diseases are still a major health burden worldwide and the increase of antimicrobial resistance to current therapies poses a serious threat for their eradication. The session will focus on new targets and new approaches to tackle these important challenges.

Keynote: **Bill Hunter** (University of Dundee)

Targeting pterin metabolism in Trypanosomatids: sobering lessons

16:35 – 18:05

Order/Disorder (PCG)

Chair: Helen Playford (ISIS)

Structural disorder can be a material's defining feature. It can influence properties and applications, and change our understanding of fundamental physics. This session celebrates the order within disorder, with potential topics including (but not limited to): the structure of nanomaterials, single crystal diffuse scattering, pair distribution function analysis, self-assembly, low-dimensional materials, disordered magnetism, materials with anomalous physical properties, and so on. Studies that illustrate the challenges of dealing with complex materials are particularly welcome in this session.

Keynote: **Matthew Blunt** (UCL)

Two-dimensional molecular networks: from random tilings to covalent-organic frameworks

Helen Duncan (Queen Mary)

Using the reverse Monte Carlo method and total scattering to model disorder in ferroelectrics

Moreton Moore (Royal Holloway)

Optical and X-ray topographic studies of dislocations, growth-sector boundaries and stacking faults in synthetic diamonds

Mark Senn (University of Oxford)

Emergence of long-range order in BaTiO₃ from local symmetry-breaking distortions

16:35 – 18:05

Chemical Insights from Charge Density (CCG)

Chairs: Hazel Sparkes (University of Bristol), Graham Tizzard (University of Southampton)

The session will examine approaches to obtain insights into chemical processes and properties through analysis of the electron density. The aim is to include results obtained using both experimental X-ray diffraction data and theoretical methods such as charge density analyses, Hirshfeld surfaces or PIXEL calculations to obtain a more detailed understanding of the charge distribution in the crystal structure.

Keynote: **Simon Parsons** (University of Edinburgh)

The role of electron density in structure interpretation

Lucy Mapp (University of Southampton)

Understanding pharmaceutical co-crystal properties via charge density

Jamie Platts (University of Cardiff)

Claire Wilson (University of Glasgow)

16:35 – 18:05

Extracellular Matrix and Cell Adhesion (BSG)

Chair: Jordi Bella (University of Manchester)

This session will focus on recent developments on the structural biology of extracellular matrix proteins and cell adhesion molecules including crystallographic analysis of their biosynthesis and molecular assembly mechanisms, processing, secretion and extracellular matrix deposition, and cell-extracellular matrix interactions.

Keynote: **David Hulmes** (CNRS, Lyon)

18:15 – 19:00

PCG Plenary

Sharon Ashbrook (University of St. Andrews)

Investigating disorder and dynamics in solids using NMR spectroscopy

continued overleaf >



Wednesday 12 April, 2017

08:45 – 09.30

IG Plenary

David Rugg (Rolls Royce)

Crystallography for aerospace and nuclear sectors: an industrial perspective of the next decade

10:15 – 11:45

Phase Transitions (IG/CCG)

Chairs: Tony Bell (Sheffield Hallam University; IG), Katharina Edkins (University of Durham; CCG)

The session will discuss phase transformations, including characterisation techniques and associated modelling. The aim is to discuss a broad range of chemical and materials systems under a variety of environmental conditions. Relevant abstracts are invited from all areas of the community.

Keynote: **Quanshun Luo** (Sheffield Hallam University)

Alexander Cousen (University of Bath)

Preparation, characterisation and preferential crystallisation of enantiomeric multi-component materials (MCMs): the case of naproxen and 2-aminopyridine

Jona Foster (University of Sheffield)

Liquid exfoliation of functionalised layered metal-organic frameworks to nanosheets

Željko Skoko (University of Zagreb)

One step closer to solving a mystery: structural and theoretical study of the thermosalient phenomenon

10:15 – 11:45

Complementary Techniques (CCG/PCG)

Chairs: Elliot Carrington (University of Sheffield; CCG), Emma McCabe (University of Kent; PCG)

Significant developments have recently been made to characterise crystalline and non-crystalline materials using techniques other than diffraction. Such methods are often especially valuable for materials whose behaviour is affected by local structure or disorder. The session will focus on complementary characterisation methods such as spectroscopy, and insights from theory and physical properties, including work from both chemical and physical crystallography backgrounds.

Keynote: **Paul Hodgkinson** (University of Durham)

Using NMR and first-principles calculation to understand disorder in molecular organic solids

Christopher Jones (University of Durham)

Just add water: exploiting hydration to unlock new self-assembly pathways

Michael Warmby (Diamond Light Source)

Bend it like Bragg: understandable reversible amorphous to crystalline phase transitions in MOFs

Cory Widdifield (University of Durham)

Crystal structure databases and NMR crystallography: the potential for structure distinctions and verifications of organics

10:15 – 11:45

Multidisciplinary Protein Structural Analysis (BSG)

Chair: Clair Baldock (University of Manchester)

Understanding the structure-function relationships of complex biological systems usually requires data obtained from several structural techniques that provide complementary insight into the biological problem. This session will look at recent developments on the combination of crystallographic analysis with techniques such as small angle X-ray scattering, NMR, electron microscopy or electron paramagnetic resonance, amongst others.

Keynote: **Stephen Muench** (University of Leeds)

15.30 – 17.00

Crystallography of Minerals and Planets (PCG)

Chair: Anthony Phillips (Queen Mary)

Crystals are ubiquitous throughout our world and beyond it; we will focus in this session on the many applications of crystallography to Earth and planetary science. This might include experimental and computational studies of structure under geological conditions, at extremes of temperature and pressure; analysis of minerals with terrestrial or extra-terrestrial origins; and even remote crystallography from space missions.

Keynote: **Simon Redfern** (University of Cambridge)

From ångstroms to astronomical units: understanding planetary processes from the atoms up

Matthew Dunstan (University of Cambridge)

Combined in silico and experimental screening of materials for carbon capture

Dominic Fortes (ISIS)

Metastable mineralogy of quenched cryomagmatic liquids

Anna Herlihy (Diamond Light Source)

Thermal processing of interstellar silicate analogues

15.30 – 17.00

Multi-Component Crystals (CCG)

Chairs: Gareth Lloyd and Hayley Green (Heriot-Watt University)

The session aims to highlight research on multi-component crystalline systems including co-crystals, solvates, hydrates, and inclusion compounds. Of particular interest is understanding structure-property relationships in such materials through their design and characterisation.

Keynote: **Krešo Bučar** (UCL)

Engineering molecular crystals: backbreaking, yet gratifying

Nick Blagden (University of Lincoln)

Crystal growth considerations for crystal engineering

Katerina Edkins (University of Durham)

Substituent influence on self-assembly of pharmaceutical drug compounds

Charlie McMonagle (University of Edinburgh)

Gas uptake within fullerene-stabilised phthalocyanine nanoporous molecular crystals

15.30 – 17.00

Advances and Challenges in Drug Discovery (BSG)

Chair: Martin Noble (University of Newcastle)

Recent years have brought the development of different approaches in drug development leading to more specific and sophisticated targeted therapies. Structure-based fragment methodologies together with protein-protein interaction inhibitors are now generating new opportunities for drug development. The session will focus on new advances and challenges in drug discovery and how structural analyses support their development.

Keynote: Rod Hubbard (University of York)

17:10 – 18:00

Bragg Lecture

Mike Glazer (University of Oxford)

The wondrous world of perovskites

Thursday 13 April, 2017

08:45 – 09:30

BSG Plenary

James Naismith (University of St. Andrews)

The structural biology of natural product biosynthesis

10:15 – 11:45

New Insights into Old Problems (PCG)

Chair: Mark Senn (University of Oxford)

The session aims to present work that brings new structural insights into long-standing problems, where new methodology or unconventional techniques have been used to tackle problems which have conventionally been viewed as insoluble or, where the study of new materials has led to old problems being re-evaluated. Abstract submission is encouraged from a broad range of scientific areas.

Keynote: Abbie McLaughlin (University of Aberdeen)

The structure and electrical properties of complex hexagonal perovskites

Abbey Jarvis (University of Birmingham)

Introduction of oxyanions in perovskite and related systems

Lewis Owen (University of Cambridge)

Analysis of short-range order in Cu₃Au using X-ray pair distribution functions

Carl Romao (University of Oxford)

Elastic and vibrational origins of thermal expansion anisotropy in flexible molecular frameworks

10:15 – 11:45

Extended Materials (CCG)

Chairs: Helena Shepherd (University of Kent), Jonathan Foster (University of Sheffield)

Designing and synthesising extended materials with a desired topology remains an outstanding challenge in crystal engineering. Understanding how to control the assembly, and

ultimately the properties, of such materials requires insights from a wide range of techniques alongside crystallography. The session welcomes contributions from speakers working with a diverse range of materials.

Keynote: Neil Champness (University of Nottingham)

Alistair Overy (University of Oxford)

Extreme cooperative swelling in topologically disordered fibre entanglements

Seth Wiggins (CCDC)

Knowledge-based approaches to metal-organic frameworks

Tim Easun (University of Cardiff)

10:15 – 11:45

Tackling Cancer: New Approaches to Therapy (BSG)

Chair: Aude Echalier (University of Leicester)

Cancer is a multifactorial complex set of diseases that respond to a number of environmental and intrinsic factors. Understanding the molecular basis of different types of cancer is essential to progress towards better treatments. The session will focus on new potential targets for cancer therapy as well as recent advances on the development of protein inhibitors of known targets.

Keynote: Jane Endicott (University of Newcastle)

CDK structures reveal unique and conserved features: lessons for drug design

12:00 – 13:30

Distortion and Dynamics (PCG)

Chairs: Jan-Willem Bos (Heriot Watt University) and Nick Funnell (ISIS)

This session arises from common themes drawn from submitted abstracts. Structural mobility and flexibility underpins much of the world of functional materials, whether this be subtle distortions of polyhedra or large-scale atomic/ionic mobility through a crystal lattice, that ultimately gives rise to function. This session aims to highlight such materials and means by which we measure and model their structures.

Keynote: Phoebe Allan (Diamond Light Source)

Lithium and sodium storage mechanisms in alloying anodes for rechargeable batteries: insights from local structure characterisation

James Cumby (University of Edinburgh)

Gaining insight from polyhedral distortion

Anthony Philips (Queen Mary)

Cation dynamics in framework materials

12:00 – 13:30

Would You Publish This? (CCG/YCG)

Chairs: William Lewis (University of Nottingham; CCG), Claire Hobday (University of Edinburgh; YCG)

This interactive session will discuss problematic crystal structures that can be hard to interpret and publish. After the opening keynote talk, the session is open for anyone to describe structural results that raise the session title question. The audience will discuss, with the aim to provide constructive

advice. Problems might include charge imbalance or other chemical issues, poor resolution or data completeness, complicated disorder, highly restrained models, unexplained residual electron density, etc. A formal abstract is not required, but please contact the session organisers in advance of the meeting (as soon as possible!) if you wish to contribute; 1-3 slides will be requested for concatenation into a single session presentation. Contributions from YCG members are particularly encouraged.

Keynote: Iñigo J. Vitórica-Yrezábal (University of Manchester)
Is it or is it knot publishable?

12:00 – 13:30

Multiprotein Complexes (BSG)

Chair: Steve Prince (University of Manchester)

Multiprotein complex formation is at the centre of critical biological processes such as macromolecular assembly, receptor-ligand recognition, or host-pathogen interactions. Crystallographic analysis of these complexes remains a challenging problem due to technical complexity that starts at the molecular biology level and extends all the way to the structure determination. This session will look at recent representative examples of crystallographic analyses of multiprotein complexes, the difficulties encountered, and the approaches taken to overcome them.

Keynote: Mark Banfield (John Innes Centre)
Neutralising cereal killers: engineering plant immune receptors to help feed the world

Workshops

Please refer to the meeting website for up-to-date workshop details: <http://bcaspringmeetings.org.uk>.

Programme Committee

Chair: Andrew Bond (University of Cambridge).

BCA: Lee Brammer (University of Sheffield), Richard Cooper (University of Oxford).

BSG: Lydia Tabernero (University of Manchester), Jordi Bella (University of Manchester).

CCG: Gareth Lloyd (Heriot-Watt University), William Lewis (University of Nottingham).

IG: Ghazala Sadiq (CCDC), Helen Blade (AstraZeneca)

PCG: Nick Funnell (ISIS), Jan-Willem Bos (Heriot-Watt University).

YCG: Sam Horrell (University of Essex), Claire Hobday (University of Edinburgh).

Workshops: Horst Puschmann (OlexSYS), Nick Funnell (ISIS)

Organisers: Joanne McBratney, Nicola Hardaker (Hg3 Conferences).

Puzzle Corner



Answer to December Puzzle Corner

¹ E	U	² R	O	P	³ E	::	⁴ A	⁵ R
P	::	A	::	::	⁶ G	A	L	E
::			::	::				
⁷ S	⁸ A	N	⁹ T	¹⁰ A	::	::	¹¹ S	I
					::	::		
¹² R	A	D	I	A	T	¹³ I	O	N
C	::	¹⁴ O	N	::	::	R	::	D
::	¹⁵ A	M	::	¹⁶ O	¹⁷ S	::	¹⁸ N	E
::			::			::		
¹⁹ S	N	::	²⁰ A	P	P	²¹ Y	::	E
		::						
::	²² N	²³ E	W	::	²⁴ Y	E	²⁵ A	R
::				::				
²⁶ P	O	L	E	::	::	::	L	::
				::	::	::		

Across

- Continent drifting apart from the UK (6)
- Element forming some crystalline clathrates, more common than the one in September CN (2)
- Strong wind (4)
- Bringer of seasonal gifts (5)
- Found in all silicates (2)
- X-rays, visible light, etc. (9)
- Main power switch position required to generate 12 (2)
- Morning time (2)
- Naturally occurring element with the greatest density (2)
- Element that recently formed its first crystalline clathrate, reported in September CN (2)
- Symbol for 9 (2)
- 20, 22, 24. What you wish a Cockney or a smartphone on January 1 (4, 3, 4)
- Where 7 has his headquarters (4)

Down

- Bringer of scientific gifts (5)
- Not systematic (6)
- For example (1.1.)
- In addition (4)
- Animals that help 7 (8)
- Hawaiian term for a type of basalt lava (2)
- Element used for coating cans (3)
- Hawaiian term for a type of basalt lava (2)
- Type of 12 (2)
- New year will be ???? Domini 2017 (4)
- Short for a surgeon's work (2)
- What children shouldn't do when 7 comes (3)
- What we feel when contemplating a beautiful crystal structure like the ribosome (3)
- God rest ?? merry gentlemen (2)
- Short for an elevated railway (2)
- Element used in aircraft (and a flying sleigh?) (2)

Invitation to come to IUCr2017

Gautam R. Desiraju

Immediate Past President, IUCr

Solid State and Structural Chemistry Unit, Indian Institute
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Chairman, Local Organizing Committee, International
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@GautamDesiraju

I AM writing this specifically to my colleagues and friends in the United Kingdom. The international program committee for IUCr2017 met in Hyderabad in March 2016 and has mapped out a program of three plenary lectures, 40 keynote lectures and 119 microsymposia in nine parallel sessions.

For the first time, the IUCr is proactively involved in setting up the program in the form of a keynote lecture and around six microsymposia in what are termed 'special activities', subjects that are of unique interest to the Union itself. These involve sessions devoted to data deposition, crystallographic dictionaries and nomenclature, and outreach activities into small countries, a direct spin-off from the very successful International Year of Crystallography.

State of the art, highly convenient facilities at the HICC convention center will ensure the smooth running of the conference. Posters, lunch and exhibits will be in the same large hall. Electronic posters are planned and electronic abstracts with links to IUCr journals will be freely available throughout the Congress. All IUCr journals will be freely available within the Congress venue.

The Novotel, a five star hotel attached to the convention center has 220 rooms starting at GBP 140, inclusive of all taxes. Many 4- and 5-star hotels are within 2 km of the convention center, belonging to well-known international and Indian chains with rooms from GBP 40 upwards (see web site). Shuttle buses are planned that will run between major hotels and the conference venue to a fixed time schedule. Taxis will also be available outside the conference venue for reasonable rates throughout the day. Combined accommodation and registration packages for students will be priced very reasonably, around GBP 300 for the entire duration of the Congress.

Hyderabad is a safe city. Remaining within the confines of the venue and opting for guided city tours arranged by the organizers will keep you safer. A hot (in temperature, but completely non-spicy) lunch prepared at five star standards by the Novotel for all the days of the conference is included in the registration and will be served in the exhibition/poster area.



Hyderabad is easily accessed as it is a centrally located city. London Heathrow, London Gatwick non-stop to Delhi (7 hours) or Mumbai (8 hours) and then a 1.5 hour flight to Hyderabad is a convenient option. British Airways flies non-stop to Hyderabad from London Heathrow (9 hours). Alternatively, you can use one of the Gulf airports as a hub. Easy air access from Hyderabad is possible to popular tourist destinations within India like Agra, Delhi, Jaipur, Mumbai, Kolkata, Chennai and Goa for sightseeing before and after the conference.

I am writing several letters to crystallographers in several countries, but this one written to you in the United Kingdom is of course different and special for reasons that do not really need to be spelled out. Ever since 1603, when Sir Thomas Roe came to the court of Emperor Jahangir, our countries have been united in a relationship that has been commented, discussed and debated in many forums all over the world over the centuries. Recent years have seen a real change in India and it is my earnest wish that as many friends and well-wishers of this country from the United Kingdom do visit us and personally see what is happening in India as a whole and especially in the world of science and crystallography.

See you in Hyderabad!

Gautam R. Desiraju

Microsymposia at IUCr-2017

Biological Macromolecules (Function)

MS-009	Enzymes, mechanism and drug design	22 August 2017	1030-1305
MS-018	Ion transport	22 August 2017	1455-1730
MS-027	Engineered proteins for industry and medicine	23 August 2017	1030-1305
MS-036	Structural immunology and receptor signalling	23 August 2017	1455-1730
MS-054	Mechanisms of bacterial resistance	24 August 2017	1455-1730
MS-063	Cell signalling, ubiquitination and cell death	25 August 2017	1030-1305
MS-072	Solving the phase problem without experimental phasing	25 August 2017	1455-1730
MS-081	Macromolecular machinery	26 August 2017	1030-1305
MS-090	Spectroscopy applications in biologically relevant systems	26 August 2017	1455-1730

Biological Macromolecules (Structure)

MS-001	Analysis and validation of protein ligand structures	22 August 2017	1030-1305
MS-010	Membrane proteins, lipid-protein interactions and membrane fusion	22 August 2017	1455-1730
MS-019	Interactions between proteins and nucleic acids	23 August 2017	1030-1305
MS-028	Long wavelength applications in macromolecular crystallography	23 August 2017	1455-1730
MS-037	Macromolecular structures by hybrid methods	24 August 2017	1030-1305
MS-046	Macromolecular structure determination at XFEL sources	24 August 2017	1455-1730
MS-055	New challenges in interpretation of structural data	25 August 2017	1030-1305
MS-064	Time and motion resolved imaging and diffraction	25 August 2017	1455-1730
MS-073	Minimizing radiation damage	26 August 2017	1030-1305
MS-082	Techniques and insights into macromolecular crystallization	26 August 2017	1455-1730
MS-091	Expression of macromolecular complexes	27 August 2017	1030-1305
MS-100	Structure determination of biological macromolecule complexes by Cryo-EM	27 August 2017	1455-1730

Crystal Engineering of MOFs & Open Framework Compounds

MS-002	Crystallographic approach for designing new metal organic frameworks	22 August 2017	1030-1305
MS-011	Applications of post-synthesis modified metal-organic frameworks	22 August 2017	1455-1730
MS-020	Controlling dimensions of porous crystalline polymers	23 August 2017	1030-1305
MS-029	Porous framework materials for gas adsorption	23 August 2017	1455-1730
MS-038	Porous framework materials for separation	24 August 2017	1030-1305
MS-047	Crystalline materials characterization with combined techniques	24 August 2017	1455-1730
MS-056	Direct observation of reactions and labile species within porous frameworks	25 August 2017	1030-1305
MS-065	New structures for natural and synthetic open framework materials	25 August 2017	1455-1730
MS-074	Porous framework materials for catalysis and renewable energy	26 August 2017	1030-1305
MS-083	Polyoxometalates as building blocks for functional materials	26 August 2017	1455-1730
MS-092	Bio-compatible porous materials for drug delivery	27 August 2017	1030-1305
MS-101	Porous framework materials for sensing	27 August 2017	1455-1730
MS-110	Phase transition in alloys and molecular solids	28 August 2017	1030-1305
MS-119	Interactions in solids under stress	28 August 2017	1455-1730

Crystal Engineering of Organic & Pharmaceutical Compounds

MS-003	Crystal engineering solutions to improve pharmaceutical tabletting	22 August 2017	1030-1305
MS-012	Structure-property correlation in pharmaceutical solids	22 August 2017	1455-1730
MS-030	Crystallization mechanisms of small molecule organic materials	23 August 2017	1455-1730
MS-039	Structural chemistry in 2-D: Crystal growth, surface structure and morphology	24 August 2017	1030-1305

MS-048	Supramolecular synthons at the confluence of theory and practice	24 August 2017	1455-1730
MS-057	Charge density studies in crystal and cocrystal engineering	25 August 2017	1030-1305
MS-066	Bending, jumping and rotating: Motion and movement in crystalline solids	25 August 2017	1455-1730
MS-075	Tailored properties of molecular co-crystals	26 August 2017	1030-1305
MS-084	Soft organic and inorganic materials: Gelation and crystallization	26 August 2017	1455-1730
MS-093	Halogen bonding in crystal engineering	27 August 2017	1030-1305
MS-102	Halogen bonding at the interface between small molecules and macromolecules	27 August 2017	1455-1730
MS-111	Structural chemistry at non-ambient conditions	28 August 2017	1030-1305
MS-115	Polymorphism and structural transformations in crystalline materials	28 August 2017	1030-1305

Instrumentation techniques and/or Computation

MS-004	Novel direct methods for electron diffraction and imaging	22 August 2017	1030-1305
MS-005	Total scattering	22 August 2017	1030-1305
MS-006	Computational materials design	22 August 2017	1030-1305
MS-013	Quantitative electron imaging and tomography	22 August 2017	1455-1730
MS-014	Advanced neutron sources in biological and materials sciences	22 August 2017	1455-1730
MS-015	In-situ and in-operando characterization of energy materials	22 August 2017	1455-1730
MS-022	Surface reactivity in inorganic and magnetic materials	23 August 2017	1030-1305
MS-023	Synchrotron and XFEL for materials at ambient and extreme conditions	23 August 2017	1030-1305
MS-024	NMR Crystallography and related methods	23 August 2017	1030-1305
MS-031	Nanoparticles / nanostructures	23 August 2017	1455-1730
MS-033	Magnetic diffuse scattering and magnetic PDF analysis	23 August 2017	1455-1730
MS-040	Microstructure, defects, stress and strain determination and modelling with powder diffraction data	24 August 2017	1030-1305
MS-041	Advances in computational methods for powder diffraction	24 August 2017	1030-1305
MS-042	High-resolution spectroscopy	24 August 2017	1030-1305
MS-049	In-situ and in-operando characterization of catalytic and functional materials	24 August 2017	1455-1730
MS-050	Small-Angle Scattering studies of biomacromolecular kinetics	24 August 2017	1455-1730
MS-051	Recent developments in XAFS spectroscopy: Theory, instrumentation and data analysis	24 August 2017	1455-1730
MS-058	Powder diffraction & polymorphism. Search, phase transformations and new polymorph identification	25 August 2017	1030-1305
MS-059	Quantitative electron diffraction	25 August 2017	1030-1305
MS-060	XAS at extreme conditions	25 August 2017	1030-1305
MS-067	Grain mapping and spatially-resolved diffraction – reaching the ppm scale	25 August 2017	1455-1730
MS-068	New X-ray sources: Storage rings – FELs- laser-based	25 August 2017	1455-1730
MS-069	High-pressure crystallography as the ultimate interdisciplinary tool	25 August 2017	1455-1730
MS-076	Diffuse scattering in crystalline structures	26 August 2017	1030-1305
MS-077	Coherence, spectroscopy and time resolved crystallography with new sources	26 August 2017	1030-1305
MS-078	Advances in high-pressure crystallographic methods	26 August 2017	1030-1305
MS-085	Dynamic phenomena and material functionality from inelastic x-ray scattering	26 August 2017	1455-1730
MS-086	Accurate high resolution diffraction studies at high pressure	26 August 2017	1455-1730
MS-094	Phase-plates: Improving resolution in CryoEM	27 August 2017	1030-1305
MS-096	XAFS of materials for clean energy	27 August 2017	1030-1305
MS-103	Methods for characterizing commensurate and incommensurate magnetic structures	27 August 2017	1455-1730
MS-105	New instrumental developments for electron crystallography	27 August 2017	1455-1730
MS-112	Laboratory sources vs. large scale facilities for charge density studies	28 August 2017	1030-1305
MS-121	Synchrotron-based X-ray techniques and the environment	28 August 2017	1455-1730

Materials and Minerals

MS-007	Topology and symmetry of modular structures	22 August 2017	1030-1305
MS-025	Crystallography of battery materials	23 August 2017	1030-1305
MS-034	Synthesis and properties of multi ferroics and multi-functional materials	23 August 2017	1455-1730
MS-052	Minerals/gems in industrial applications	24 August 2017	1455-1730
MS-061	Perovskites, perovskites and perovskites!	25 August 2017	1030-1305
MS-070	Superconducting materials	25 August 2017	1455-1730
MS-079	Topological insulators	26 August 2017	1030-1305
MS-088	Hybrid perovskites	26 August 2017	1455-1730
MS-097	Functional magnetic materials	27 August 2017	1030-1305
MS-106	Functional materials on the nanoscale	27 August 2017	1455-1730
MS-108	Charge and spin density in molecular and supramolecular magnets	27 August 2017	1455-1730
MS-122	Crystallography of materials for energy	28 August 2017	1455-1730

Physical and/or Fundamental

MS-008	Magnetic order and its consequences	22 August 2017	1030-1305
MS-017	Extending the boundaries of crystallography	22 August 2017	1455-1730
MS-026	A bridge between two worlds: Graphs as structural descriptors	23 August 2017	1030-1305
MS-035	Crystal structure relationships and their applications	23 August 2017	1455-1730
MS-043	Models for refining the electron density from elastic scattering – Bob Stewart's legacy	24 August 2017	1030-1305
MS-062	Topological magnetic structures: monopoles, skyrmions, etc.	25 August 2017	1030-1305
MS-089	Chemistry and physics of modulated and composite crystals	26 August 2017	1455-1730
MS-098	Recent advances in quasicrystal research	27 August 2017	1030-1305
MS-123	Magnetic structures at extreme conditions	28 August 2017	1455-1730
MS-124	Beyond conventional topological analysis of electron density	28 August 2017	1455-1730
MS-125	Small-Angle Scattering data formats, standards and repositories	28 August 2017	1455-1730

Special Activities

MS-016	New approaches in crystallographic teaching	22 August 2017	1455-1730
MS-021	Terminology issues in crystal engineering	23 August 2017	1030-1305
MS-032	Crystallography courses around the world	23 August 2017	1455-1730
MS-044	Structural databases as teaching tools – Part A (macromolecules)	24 August 2017	1030-1305
MS-045	Structural data bases as teaching tools – Part B (organics, minerals)	24 August 2017	1030-1305
MS-053	Scientific value of raw data	24 August 2017	1455-1730
MS-071	Crystallographic patterns in art and cultural heritage	25 August 2017	1455-1730
MS-080	Emerging science in the emerging world	26 August 2017	1030-1305
MS-087	How does crystallography help you in your career?	26 August 2017	1455-1730
MS-095	Crystallography for Space Sciences	27 August 2017	1030-1305
MS-099	Crystallographic data and structure validation from data collection to publication – IUCr setting standards	27 August 2017	1030-1305
MS-104	Synchrotron measurement in conservation and cultural heritage	27 August 2017	1455-1730
MS-107	Robust programming for CIF, NeXus, and related file structures	27 August 2017	1455-1730
MS-109	CryoEM: Method of the decade	28 August 2017	1030-1305
MS-113	Anticipating the Harvest: Post IYCr	28 August 2017	1030-1305
MS-114	Crystallography and cultural heritage: From microsampling to noninvasive techniques	28 August 2017	1030-1305

BCA – BSG / CCG / IG Group Meetings 2016

Biological Structures Group (BSG) Meeting 2016



THE BCA Biological Structures Group winter meeting entitled 'Seeing the Wood for the Trees in Structural Biology' was held on Monday December 19th 2016 at Birkbeck College London. In the first session, chaired by Dr Mark Roe (Sussex), Prof Tom Blundell (Cambridge) began the meeting with a talk entitled '*Increasing complexity to obtain selectivity in cell regulation*' in which he addressed the question of why molecular complexity is important for drug discovery. Prof Blundell described how his interest in structural biology began while working for the Nobel prize-winner Dorothy Hodgkin in Oxford on crystals of insulin and how he was able to establish a new laboratory at the University of Sussex in 1972 with a team including Steve Wood. During the subsequent 4 years in Sussex his team published 3 Nature papers, mainly concentrating on polypeptide hormones. Tom described one of his early studies on insulin from hystricomorphs (rodents such as rats and porcupine) which addressed the question of whether evolution of insulin is Darwinian or not. His work in that era included studies of the hormone glucagon which, together with insulin, is intricately involved in the yin and yang of blood glucose control. A key structure, that of the nerve growth factor NGF1, which

took some 15 years to solve, was determined in 1991 at Birkbeck where Prof Blundell's team was based between 1977 and 1996. He described how his interest in receptor activation and signal transduction led him to Cambridge where, amongst many discoveries, his team have unravelled the mechanism of fibroblast growth factor (FGF) receptor clustering, firstly by formation of weak dimers followed by further cooperative binding events. Such complex systems, where a protein may be as large as 4000 amino acids, are studied by mass-spectrometry, small-angle X-ray scattering (SAXS) and cryo-electron microscopy which has revolutionised the structural biology field. Databases are employed for predicting protein-ligand and multi-protein complexes and site-directed mutagenesis can be used to confirm predicted interactions. Tom concluded his talk with a description of cyclin-dependent kinase (CDK) fragment screening to discover drugs targeting protein-protein interactions.

Prof Garry Taylor (St Andrews) then gave a lecture entitled '*An engineered multivalent sialic acid binding biologic as a preventative of influenza*' in which he first described how he started working for Prof Blundell at Birkbeck in 1978 as a post-doctoral researcher where he met Steve Wood. Garry mentioned how he currently organises the BCA protein crystallography summer school in St Andrews. One focus of his current work is on viral sialidases with a special interest in *Vibrio cholerae* sialidase. Having identified ligands with around 20 µM potency, current collaborative work includes trying to polymerise them to increase avidity as potential antiviral drugs. Another aim of current work is to engineer carbohydrate binding module (CBM) proteins to bind to viral sialidase receptors on the host cell to block viral infection. These have been found to work *in vivo*. Another main interest of Garry's work is the sialidase from *Pseudomonas aeruginosa* and in making multivalent CBMs which have been shown to be very effective in protecting mice from flu infection, both as a



Speakers and chairs. From left to right: Helen Saibil, Simon Kolstoe, Vilmos Fulop, Liz Carpenter, Laurence Pearl, Steve Wood, Tom Blundell, Mark Roe, Kate Brown, Jonas Emsley and Neil MacDonald.

preventative and in immunising them against further infection by other flu strains. The multivalent CBMs have been found to increase cytokines in the lungs, so in addition to masking the viral receptor, they also stimulate the immune system. Their potential for treatment of other respiratory infections and pandemics has led to a spin-out being started.

Prof **Helen Saibil** (Birkbeck) then gave a talk entitled '*Protein aggregation, chaperones and disaggregation*' in which she described the development of one of the first projects that she worked on at Birkbeck in the early 1990's which began as a collaboration with Steve Wood. This is the chaperonin GroEL, which has been studied by hybrid tomography and more recently at the new Diamond facility. The protein is a large assembly of subunits and possesses a polar cavity in which the unfolded ligand protein can renature. Helen described how recent studies have allowed the complex of GroEL with a bacteriophage protein gp31 bound in the core to be characterised. The binding of ATP to GroEL gives a range of conformations in which the mouth of the protein is opened to different extents. She is currently working on the chaperone Hsp70 and how it reverses protein aggregation with cofactors Hsp40 and Hsp110. Proteins are unfolded by being pulled through the middle of this large complex. The neuronal protein alpha-synuclein is of particular interest. Other studies include the threading of unfolded protein substrates through the ClpB/Hsp104 disaggregase and proteasomes – systems which use six-membered rings of AAA subunits to thread the protein substrate into the channel for ATP-dependent degradation.

Next up, **Patrick Shaw-Stewart** of Douglas Instruments gave a presentation entitled '*Microseed matrix-screening (rMMS): introduction, theory, practice and a new technique for membrane protein crystallization in LCP*'. Patrick described how a hit from a crystallisation screen can be used to make a seed-stock in well solution which is added back to a new random screen. This way one can get many more hits with all crystallisation methods including lipidic cubic phase (LCP).

In the first session after lunch, which was chaired by Prof **Vilmos Fulop**, Prof **Liz Carpenter** (Structural Genomics Consortium, Oxford) gave a presentation entitled '*Structures of human ion channels, TREKs and TRPs, by X-ray, xFEL and cryoEM*'. Liz began with a telling comparison of cloning and sequencing technologies in the 1980's with those available today. Her current work involves studies of human proteins in which insect cell lines are used for screening a large number of expression constructs, typically 12 - 24 per target. Liz described work on K2P ion channels which are potassium channels with two pore-forming helices that are important regulators of cellular electrical excitability. The structure of TRK2 has been solved by her group showing that the K⁺ ions are held by carbonyl groups as they move through the channel and the protein has a fenestration for the drug norfluoxetine (prozac). TRK1 has also been solved using xFEL, a source 10¹⁰ times stronger than Diamond, with the crystals delivered to the beam in LCP. The structure of a protein involved in polycystic kidney disease (PKD2) has also been determined at 4 Å resolution using EM which gave a better map than the X-ray one showing that the protein has a novel extracellular TOP domain.

Prof **Laurence Pearl** (Sussex) then gave a presentation entitled '*Phosphorylation dependent assembly of the DNA Damage Response*' covering the BRCA1 repair complex which is as large as a single bacterium. The structure of Crb2 and a phosphopeptide complex was described along with the assembly of the 9-1-1 checkpoint clamp. The protein

Rad4(TopBP1) with which Crb2 interacts facilitates activation of the DNA damage checkpoint, the initiation of DNA replication and recombinational repair.

Prof **Neil MacDonald** (Francis Crick Institute / Birkbeck) then gave a lecture on '*Dissecting and exploiting RET receptor tyrosine kinase signalling*'. He began by describing work which he had done with Steve Wood in the early 1990's to determine the structure of nerve growth factor (NGF). Neil then described structural studies of the cadherin-based tyrosine kinase RET which is involved in development of the kidney and the enteric nervous system. Since inappropriate activation of RET signalling can lead to neoplasias, monoclonal antibodies or DARPins (genetically engineered antibody mimetic proteins) which inactivate RET are being developed as potential cancer therapies. The zebrafish protein has been analysed and shown to have 4 cadherin domains.

Marcus Winter then gave a presentation entitled '*Rigaku Oxford Diffraction: Advances in Crystallography*' covering their range of equipment for structural biology.

After coffee, the next final session which was chaired by Dr **Kate Brown** (Cambridge), began with Prof **Jonas Emsley** (Nottingham) who gave a lecture entitled '*Investigation of the contact system assembly and activation*' which is involved in blood clot formation. Jonas described the structure and function of the factor XI zymogen which consists of four apple domains creating a disk-like platform around the base of the fifth catalytic domain. A screen of 3 million peptides was conducted to find sequences that would bind in the apple domain pocket and 74 peptides were found, all with a DFP motif. The structures of a number of DFP-containing peptides bound to FXI in the apple domain pocket were solved and other high resolution structures determined.

Dr **Simon Kolstoe** (Portsmouth) then gave a lecture entitled '*Determining the molecular interactions of serum amyloid P component*'. He described some of the history of studies into amyloid disease including EM studies of amyloid fibres in the late 60's and subsequent fibre-diffraction which led to a beta-sheet model of the fibre structure. The protein serum amyloid P (SAP) binds to the fibres in a calcium-dependent manner changing their structure. The X-ray structure of SAP was determined in 1994 and found to be similar to that of concanavalin A. Strategies for treatment of amyloid disease include cross-linking drugs to deplete its concentration in the plasma and monoclonal antibodies. Expression of SAP in HEK cells gave large yields of protein and has allowed the DNA-binding properties of SAP to be studied by the use of Selex technology to find short oligonucleotide sequences which have high affinity for SAP. The putative DNA-binding function of SAP is corroborated by the fact that certain mutations of the protein abolish its DNA-binding ability and a physiological role is suggested by the fact that neutrophils spill out large amounts of DNA which SAP binds to during inflammation.

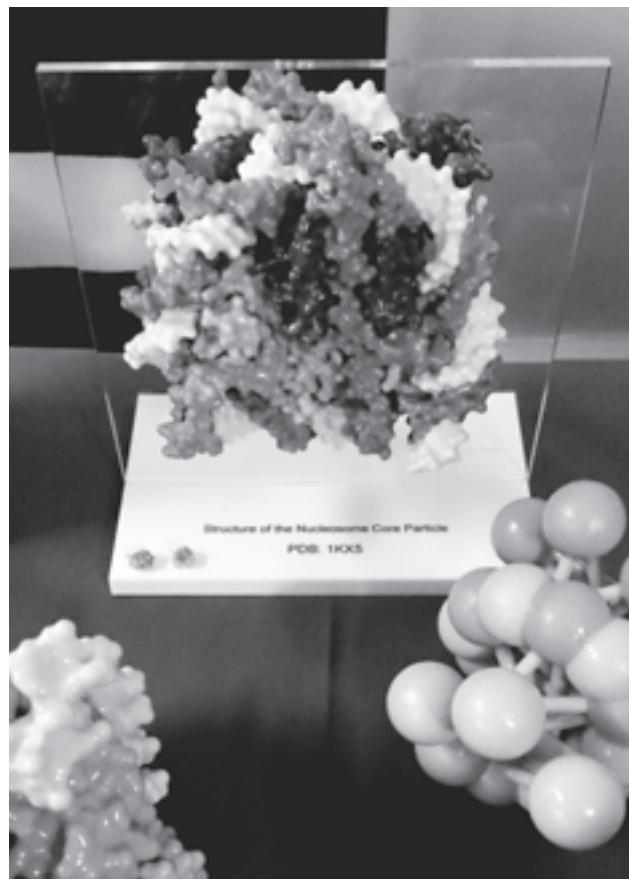
The scientific sessions ended with the award of a poster prize to **Jingxu Guo** (UCL) which was presented by **Darren Gowers** (Molecular Models / Portsmouth). A gift to **Steve Wood**: a laser-etched glass crystal showing a cross-linked drug complex of SAP was then presented by **Tony Savill** of Molecular Dimensions Ltd. Finally, the event concluded with a reunion / reception for the many ex-colleagues of Prof Steve Wood who, along with the meeting attendees are thanked for making the conference such a memorable occasion. The event was sponsored by Bruker, Douglas Instruments, Jena Bioscience, Molecular Dimensions, Molecular Models, Oxford

Cryosystems, Rigaku Oxford Diffraction & UCL Centre for Amyloidosis and Acute Phase Proteins. Professor **Nick Keep** (Birkbeck) is also sincerely thanked for excellent local organisation of the meeting.

J. Cooper and S. Najmudin

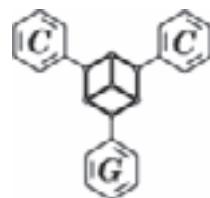


Jingxu Guo receiving poster prize from Darren Gowers.



Poster prize from Molecular Models.

Chemical Crystallography Group (CCG) Meeting 2016

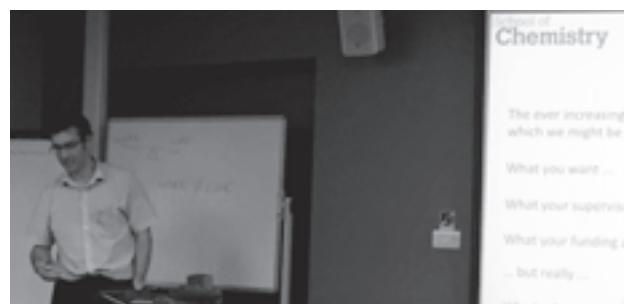


THE Annual Chemical Crystallography Group (CCG) Autumn meeting was held in Newcastle-upon-Tyne on the 16th of November 2016. This year's theme was '*Non-Ambient Crystallography*' and a fine line-up of six speakers was well appreciated by the excitable turnout of chemical crystallographers at the meeting.

After the general melee of reacquainting with old and new friends, the day was started by Dr **Pete Wood** of the CCDC. The talk focused on the "completion" of the periodic table within the CSD by determining a structure containing Neon. By utilising *in situ* gas structural powder diffraction on a series of MOFs, this story based around a multi-national collaboration, managed to bring the "missing" Neon structure to the light of day. The end of the talk brought an interesting discussion over the accuracy differences between powder and single crystal diffraction. This morning session provided insights into the "low" pressure regime of structural "Non-Ambient" crystallography. And the theme continued with the next two speakers. The morning was completed by the previous two CCDC young scientist prize winners, Dr **Mark Warren** (2016) and Dr **Nick Funnell** (2015). Both are at major facilities, Diamond and STFC, respectively, and gave excellent overviews of what we can expect to be able to do on the available beamlines and what has been done. Again, examples of *in situ* gas structure work is driving research portfolios around the country and major facilities. It is clear that many exciting results will be coming from these major facilities over the next few years.

The lunch break was lively, well-received and well-organised. Dr **Mike Probert** must be thanked for his excellent venue and value. And, of course, for the very palatable lunch.

The post-lunch session, chaired by Dr **Katharina Edkins**, took our focus away from porous crystals. The latest winner of the CCDC young scientist award Dr **Lauren Hatcher** – see the announcement in this issue – then got the afternoon off with some "Exciting" crystals. The talk presented use of photochemistry to excite materials and cause structural changes that are measureable through some ground breaking "time-resolved" crystallography. Dr Probert, for his sins as



Dr Mike Probert.



host, was roped in to complete our “non-ambient conditions” by giving an excellent talk on low temperature crystallography. His work at Durham University shows how a concerted and focused effort, even with a difficult life:work balance of academia, can result in significantly interesting new equipment and techniques in crystallography away from the major facilities.

The final session, chaired appropriately by Prof **Simon Parsons**, finished off the “non-ambient conditions” story plot line through talks on high-pressure crystallography from Dr **Iain Oswald** and Dr **Stephen Moggach**. Dr. Oswald showed us how careful analysis can reveal interesting and unexpected phases and chemistry under pressure. This included work on performing polymerisation under pressure, touching on classic topological chemistry developed by chemical crystallographers. Dr. Moggach spectacularly finished the day and brought us back to the theme of porosity. Instead of gas pressures, the understanding and knowledge gained was garnered through high-pressure crystallography (>> 100Bar). The gate-opening mechanisms of porous materials such as ZIF8 explained through this vigilant crystallography will be crucial in designing and applying porous crystalline materials to applicable impacts outside of academia.



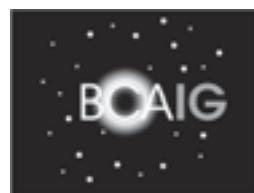
Dr Stephen Moggach.

The overall meeting showed that there is a vibrant chemical crystallography community around the country working in conditions of high pressure and variable temperature. And with this younger generation clearly showing that the subject is very much in safe hands, we all should look forward to what they will discover next.

Gareth Lloyd
Heriot-Watt University

We thank Prof Jon Steed for the photographs.

Industrial Group (IG) Meeting 2016



Autumn meeting – 10-11th November 2016

Diffracton of amorphous and disordered materials

Diamond Light Source, Oxfordshire

THIS theme of this year's Autumn IG meeting was Diffracton of Amorphous and Disordered Materials. In addition to an excellent line-up of speakers from across a range of industries, we were also lucky enough to be hosted by the new Diamond PDF beamline scientists. This meant we were treated to not only stimulating talks but also tours of the beamlines and a workshop dedicated to the practice of measuring and interpretation of Pair Distribution Functions (PDF).

After a warm welcome from the Industrial Group chair, **Chery Doherty** (Pfizer), the first session, chaired by **Helen Blade** (AstraZeneca) began with a talk from **Bruno Hancock**, also from Pfizer. Bruno outlined the properties of amorphous materials and the associated problems with characterising these materials. He also provided the audience with an insight into the drivers for the pharmaceutical industry to make use of the amorphous form of a drug but also the risks associated with this strategy.

Next we had **David Keen** from the STFC. David discussed how an amorphous phase of the metal organic framework ZIF-4 could be prepared via three different methods. He then demonstrated that through the use of PDF structural understanding could be derived for this amorphous phase using complementary scattering of neutrons and x-rays, and how the structure of the amorphous phase could be modelled from the PDF data.

The final speaker from this first session was **Katie Ryan** from SSPC, Ireland who gave a talk on strategies for enhancing the solubility of poorly soluble materials, and how strategies making use of the amorphous phase could be de-risked through encapsulation within a porous silica framework. Katie also provided the audience with an insight into the challenges of characterising the dissolution properties of such materials and demonstrating a relationship between the In-Vitro and In-Vivo tests.

The second and last session of the day was chaired by **Ghazala Sadiq** (CCDC) and was opened by **Dean Keeble**, XPDF beamline scientist at Diamond, who gave an extremely enlightening talk on the new XPDF beamline: how all aspects of the beamline had been carefully designed to maximise the quality of the PDF data it can generate. He also talked about how the DAWN software has been written with the user very much in mind to ensure that the PDFs obtained are not only robust but also removing the computational downtime a user

would experience generating PDFs from scattering data individually, through the creating of a pipeline protocol that allows users on the beamline to see and access their PDFs as soon as the data is collected.

Dean was followed by **Sheng Qi** from UEA who talked about how disorder in pharmaceuticals can not only affect the active drug molecule but also the excipients within the formulation. Sheng's research focused on understanding how the properties of an excipient(s) can affect the performance of the drug applying techniques such as thermal analysis, CT imaging and microscopy.

The final speaker of the day was **Adele Paterson** from Bristol Myers Squibb who described how in practice an amorphous drug is developed with the use of a polymer matrix, in the form of a solid dispersion. She covered the different methods of preparation and the effect on the target product profile of the material, also focussing on the methods available to quantify crystalline phases within the amorphous material.

The day ended with a series of tours of the I15-1, I11 and I12 kindly given by **Phil Chater**, **Sarah Day** and **Phoebe Allan**, followed by the conference dinner.

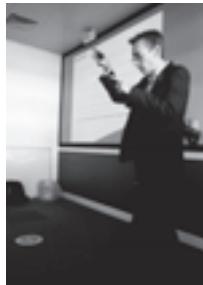
Yaroslav Khimyak from UAE was the first speaker of the second day meeting, chaired again by **Helen Blade**. Yaroslav talked us through the application of NMR for providing a structural insight into disordered materials. The use of porous Si media for preparing an in-situ stable amorphous phase was demonstrated, along with tracking co-crystal reactions and structural insights into disordered layer material.

The final talk was given by **Harry Geddes** who was the recipient of the student bursary for this meeting as a second year PhD student from Oxford University working with AstraZeneca. Harry presented on how PDF can be applied to drug – polymer formulations to offer structural understanding of the phases present and how these different components can be isolated and studied. How the structure of amorphous materials can be modelled from PDF data was demonstrated.

The meeting was concluded with an afternoon of workshops from **Phil Chater** and **Phoebe Allan** on the practical aspects of PDF taking the audience through data collection parameters and processing, providing a fantastic run-through on the use of GudrunX. This was followed by a run-through of the qualitative and quantitative aspects of analysing PDF data, including a demonstration of how to use PDFGui. The workshop and meeting was concluded with a workshop on how to model structures from the PDF data with the use of RMCprofile. A copy of the workshop material can be found on the BCA-IG website



Image taken during one of the evening's beamline tour showcasing the long duration experiments on I11.



Phil Chater,
XPDF beamline
scientist, I15-1

We thank the following for their sponsorship of the meeting: Pfizer, CCDC, Bruker and Rigaku, with special thanks going to Diamond for hosting the meeting and the significant contribution to the meeting from the beamline scientists.

Helen Blade AstraZeneca and Cheryl Doherty Pfizer

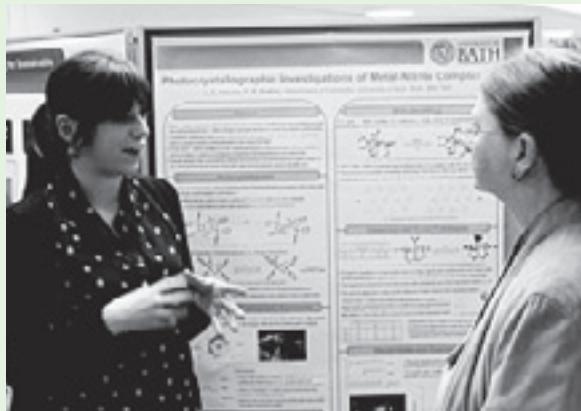
2017 CCDC Chemical Crystallography Prize

THE CCG and the CCDC are pleased to announce that the winner of the 2017 CCDC Chemical Crystallography Prize for Younger Scientists is Dr Lauren Hatcher (University of Bath). Lauren studied for a BSc in Natural Sciences at the University of Bath from 2006 to 2010, subsequently obtaining her PhD from Bath in 2014 supervised by Prof. Paul Raithby. Now she holds the post of Research Associate at the University of Bath. A session chair at a crystallography conference once facetiously introduced her as "someone who just couldn't get out of the bath"; if so, she must be the most productive occupant of the bath since Archimedes!

Lauren describes herself as primarily a crystallographer by training, whose PhD research focused on the use of non-ambient crystallographic techniques. Now, as a member of the Metastable Materials Group, a collaborative EPSRC programme that operates across the Department of Chemistry, her main research interests are in the field of photocrystallography, studying photochemical processes in the solid state using X-ray methods.



Lauren with her poster prize awarded at the meeting of the American Crystallographic Association in Hawaii in 2013, photographed by Lynne Thomas.



Lauren explaining her research on photocrystallography to the Vice-Chancellor, University of Bath (picture courtesy of the University of Bath).

Pan-African Conference on Crystallography



The participants of PCCr1 gather for a photo outside the conference venue. Picture by Bill Duax.

IT was with much excitement and some trepidation that we signed up for the first ever Pan African Conference on Crystallography (PCCr1) in Dschang, Cameroon last October. For us it was set to be a busy conference with talks, discussion sessions, chairing duties and an exhibition stand all in a country we knew very little about. But the opportunity to engage with this burgeoning community of crystallographers was too good to miss. What an experience it turned out to be on so many levels!

The trip and the conference both exceeded our expectations and were a truly memorable experience. After a restful night in Douala recovering from a flight that some of us shared with a hostile deportee (don't ask!) we ventured by bus to Dschang, which was an interesting journey not least because of the field toilets. We saw many small towns, plantations and rain forests along the way, all carefully described for us by our bilingual tour guide. Once in Dschang, we were ready for a cultural trip to the Musee des Civilisations where we learned some of the history of Cameroon followed by the opening ceremony and illuminating opening lecture by Professor **Gautam Desiraju**. We were quite pleasantly surprised to find members of the media had been invited to report on the conference which made the national news in Cameroon.

The conference itself was well attended with nearly 200 participants from over 35 different countries, with the majority of attendees coming from countries all across Africa. Being hosted by the University of Dschang it was also fantastic to see lots of students from the University at the meeting and to see so many of them actively engaged in crystallographic discussions throughout the week. Gautam started these discussions nicely by focussing on crystal engineering in his opening talk. His presentation included a look at the history of crystal engineering and what the future may bring. Perhaps most importantly, though, Gautam framed this in the context of crystallographic endeavours in the African continent and described how advancements in crystal engineering can be made even with limited resources or budgets.

The next day **Susan Bourne** and **Hocine Merazig** chaired a fascinating session that followed on from Gautam's talk and focused on crystal engineering and structural chemistry –

function though design. **Alessia Bacchi** started the session and in her talk "*Designing MOFs that breathe aromas*" she described a systematic way to embed small molecular aggregates inside porous crystalline materials. The aim of the research was to explore both the structural aspects of nanoconfinement and the stabilization of guest molecules inside the cavities of the structure. A whole host of lectures on the topic followed including "*From Cape to Alex – 15 Years of Collaboration on MOFs, Magnetism, Antimicrobials and Network Topology*" by **Lars Öhrström** that highlighted many years of collaboration with the University of Alexandria, Egypt and the University of Cape Town, South Africa, with emphasis on progress made in the analysis of crystal structures and in particular the use of network topologies.

After lunch the focus switched to Inorganic Materials and Industry Minerals and we were taken on a journey of discovery which included the design and synthesis of well-ordered nanostructured materials by **Robert Mokaya**, the growth of ZnO nanotube arrays by **Donald Tchuifon**, and the synthesis of supermagnetic Fe₃O₄ nanoparticles by **Jeremie Muswema** before finishing with a talk by **Marcia Fantini** about mesoporous zirconia based materials. The day concluded with an evening session on using crystallography as a vehicle to promote science in Africa and beyond where **Andreas Roodt** initiated discussions about the possibility of establishing an African Crystallographic Association.



(L-R) Suzanna and Amy at the CCDC stand.



Suzanna demonstrating CCDC resources to keen participants.

Over the course of the next day there were 16 talks split between two sessions. The first session focused on crystallography for life sciences with a keynote lecture from **Alejandro Buschiazzo** on “*Macromolecular Crystallography with Integrative Landscapes*”. The second session of the day covered crystallographic databases with talks on using the CSD, the ICDD and the PDB. One of the highlights of the session was a talk by **Patrice Kenflack**, a local conference organiser, who spoke about how he had used the CSD to study a new packing mode of water. Once again, the day concluded with an evening discussion session including an update on the IUCr’s OpenLab initiative and a discussion about establishing a light source in Africa.

FRANÇOISE Amombo Noa was known to followers of the CCDC as one of the researchers responsible for the 750,000th structure in the Cambridge Structural Database – announced last summer. Françoise was kind enough to send us some of her impressions of PCCr1 for inclusion in this report...

It has been an honour to be one of the participants of the “First Pan-African Conference on Crystallography (PCCr1)” held in October at the University of Dschang in Cameroon.

I was very enthusiastic the first time I heard about this conference, as Cameroon is my home country. As a PhD student doing research in South Africa at the University of Cape Town, I have had access to scientific apparatus, equipment and instruments which are not available in Cameroon.

The conference was an eye opener as it reminded me that some people in Africa do research under difficult circumstances. Many of the African scientists at the conference have to send their materials to other countries or outside the continent in order to have access to their research data because they lack necessary facilities.

It was great to see the single crystal X-ray diffractometer donated to the University of Dschang by the International Union of Crystallography (IUCr). This will help Cameroonian crystallographers to enhance their skills and to have better access to research data.

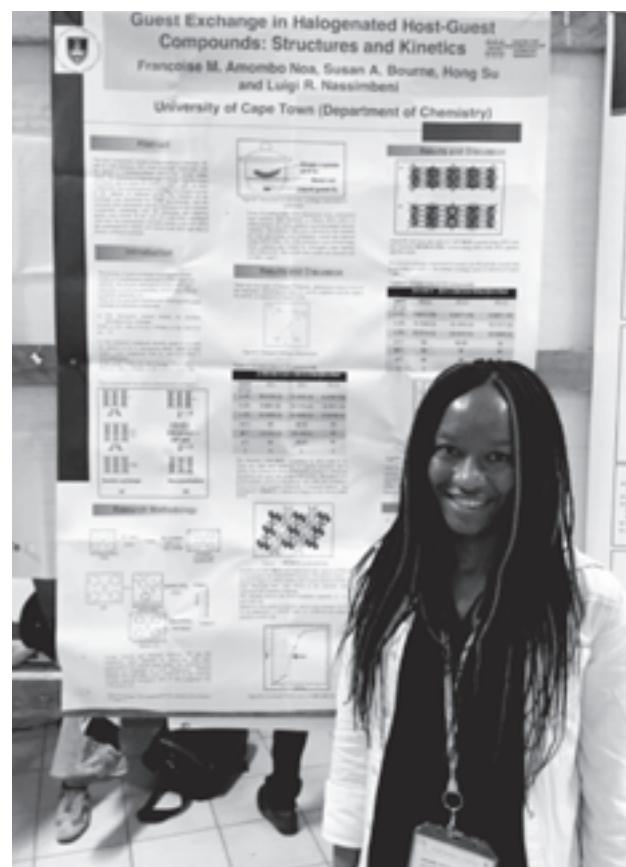
It was interesting to have the opportunity to network with participants from all over the world who have different backgrounds. *continued overleaf >*

The last full day of the conference started with a session on inorganic materials and the mining industry. This session proved highly popular to many of the conference attendees who hail from countries with major mining operations. Finally, the conference returned to where it began with the afternoon session devoted to crystal engineering.

Our final morning in Dschang brought a truly inspiring lecture from **Areej Abuhammad** who described herself as the only protein crystallographer in her country. Her journey to establish world-class research in protein crystallography in Jordan had everyone captivated. The final talk of the conference was **Ron Lifshitz**’s plenary lecture on “*What is a crystal? – New answers to an old question*” and what a fitting way to end the conference and to leave everyone with a thirst to learn more about new areas of crystallography.

It was with mixed emotions that we approached the end of the conference. It had been an extremely rewarding conference, we had had the opportunity to meet many crystallographers from across Africa for the first time and to engage with this growing community. There had been a few challenges along the way, though these simply make for entertaining stories to tell over a drink or two. I think everyone went away feeling how worthwhile the conference had been and truly a conference never to forget. It was a real pleasure to hear how crystallography was helping to advance research in so many African countries and to see how excited many of the attendees were about the prospect of using structural data in education and research at their universities for the first time as soon as they returned home.

Suzanna Ward and Amy Sarjeant
The Cambridge Crystallographic Data Centre



Françoise presenting her poster during PCCr1.

Suzanna Ward “Learning from 822,187 crystal structures” and **Amy Sarjeant** “The CSD and the weird, wonderful structures of Africa” both from the CCDC gave amazing oral presentations. Their talks had a similar orientation presenting the CSD as an invaluable tool in our research of everyday. This was particularly important because many attendees don’t have access to expensive equipment or instrumentation but they are able to access the CSD and the wealth of data in 800,000 small molecule crystal structures to further their research and understanding.

I enjoyed all other research presentations including poster sections and found some very inspiring adding to my knowledge.

Ron Lifshitz from Tel Aviv University, Israël gave an outstanding talk on quasicrystals and their lack of symmetry. In his abstract, he said *“I will review some of these profound changes in our understanding of crystallography that were brought about by the remarkable discovery of quasicrystals.”* I liked the pattern

of the pictures shown at his presentation and gained some knowledge on a topic in crystallography I know nothing about.

At the conference, I was fortunate to present a poster titled “Guest Exchange on Halogenated Host – Guest Compounds: Structures and Kinetics” (<http://dx.doi.org/10.1021/acs.cgd.5b01728>) as shown in the image on the previous page.

In this study, inclusion compounds have been utilized to store volatile halogenated guest solvents. I had the opportunity to interact, meet and talk to people I have only known by name.

The conference was a great initiative for the promotion of crystallography in Africa. This kind of meeting should be nurtured so that further development of science in Africa is encouraged.

The First Pan African Crystallography Conference in October 2016 was a success and I look forward to PCCr2!

Easier access to data deposited with CCDC

WE are pleased to announce the launch of our new web interface to allow you to view and retrieve your deposited data.

This launch builds on our online deposition service used by over 10,000 depositors annually and provides you with a new way to log in and see your previously deposited structures.

All you need to do to access your data is register and set up your user profile. You will then be able to log on and view your ‘datasets through ‘My Structures’ (<https://www.ccdc.cam.ac.uk/deposit/MyStructures>). All your deposited structures will be listed and searchable, with more detailed deposition information also available. You can also click through to visualise structures you have already published in our Access Structures service. Most importantly, you can check the status of any depositions and download and retrieve your datasets at any time. Registering for an account will also save you time when you have new data to deposit, as by logging in all your personal details will already be added to your deposit.

If you are a regular depositor you will have already seen a number of enhancements to our deposition service over the last year. These have all been in response to your feedback and have included the ability to associate multiple email address to a deposition, to automatically generate and download a 2D diagram for your deposited structures, the ability to associate your ORCID iD to your deposit and the improved handling of large datasets.

This new release is therefore just the latest addition to our deposition services and marks a significant step forward in an interactive, intuitive deposition process that can be incorporated into your daily workflows. Just like our online deposition service you can expect to see a lot of new functionality added

to this new portal over the coming months. In conversations with you, our depositors, we already know that there are a number of additional features that you would benefit from. We are therefore already working on future releases that include the ability for you to easily edit, update and maintain your structures, the ability to create in-house databases through the deposition process, the ability for you to share your structures with collaborators or across your institutions, the ability to self-assign CCDC numbers and the ability to further validate and check your structures pre-publication. We would love to hear how you would like our deposition services to develop and what your priorities are. If you have any comments or suggestions just drop us an email on web-deposit@ccdc.cam.ac.uk

More information about this new release is available on our deposition pages and we have a number of FAQs on our support pages to help answer any questions you may have.

Suzanna Ward
CCDC

Example showing the interactive table of deposited data from the ‘My Structures’ service and Example showing the Enhance Data page for our deposition service can be found on the CCDC website at:

<https://www.ccdc.cam.ac.uk/Community/blog/2016-12-01-your-deposited-data-is-now-just-a-click-away/>

Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to the list, please send them to the Editor, c.h.schwalbe@hotmail.com . Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

2-7 March 2017

ICCOSS XXIII, 23rd International Conference on the Chemistry of the Organic Solid State, Stellenbosch, South Africa.
<http://iccos2017.co.za/>

6-7 March 2017

Correlative light, electron, and X-ray microscopy symposium, Harwell.
<https://www.clf.stfc.ac.uk/Pages/Octopus-CorrelativeMicroscopySymposium.aspx>

6-8 March 2017

Towards novel therapies: Emerging insights from structural and molecular biology, Groningen, Netherlands.
<http://events.embo.org/17-structural-biol/>

6-10 March 2017

Fifth International Conference on Multifunctional, Hybrid and Nanomaterials, Lisbon, Portugal.
<http://www.hybridmaterialsconference.com/>

6-10 March 2017

Biophysics Week, various locations.
<http://www.biophysicsweek>

8-10 March 2017

Correlative light, electron, and X-ray microscopy workshop, Harwell.
<https://www.clf.stfc.ac.uk/Pages/Octopus-CorrelativeMicroscopySymposium.aspx>

13-17 March 2017

ICDD Spring Meetings, Newtown Square, PA, USA.
<http://www.icdd.com/profile/march17.htm>

13-17 March 2017

APS March Meeting 2017, New Orleans, LA, USA.
<https://www.aps.org/meetings/meeting.cfm?name=MAR17>

14 March 2017

Studying biology at cryogenic temperatures: the CryoEM revolution in structural biology, Liverpool.
<https://www.liverpool.ac.uk/events/>

16-18 March 2017

3rd Annual World Congress of Smart Materials (WCSM-2017), Bangkok, Thailand.
http://www.bitcongress.com/wcsm2017/Scientific_Programme_sm.asp

19-22 March 2017

XXIII West Coast Protein Crystallography Workshop, Pacific Grove, CA, USA.
<http://www.biochem.utah.edu/hill/wcpcw.html>

21-23 March 2017

2017 International Conference on Frontiers of Characterization and Metrology for Nanoelectronics (FCMN), Monterey, CA, USA.
<http://www2.avs.org/conferences/FCMN/>

22-24 March 2017

5th Annual Conference of AnalytiX, Fukuoka, Japan.
<http://www.bitcongress.com/Analytix2017/>

23-26 March 2017

Ninth Workshop on Structural Analysis of Aperiodic Crystals, Bayreuth, Germany.
http://aperiodic.uni-bayreuth.de/workshop_2017/

25 March – 2 April 2017

16th BCA/CCG Intensive Teaching School in X-Ray Structure Analysis, Durham.
<http://community.dur.ac.uk/durham.x-ray-school/staff.htm>

26-31 March 2017

International Workshop on Photoionization (IWP) & Resonant Inelastic X-ray Scattering (RIXS), Aussois, France.
<http://www.synchrotron-soleil.fr/Workshops/2017/IWP-RIXS2017>

27-30 March 2017

25th Annual Meeting of the German Crystallographic Society, Karlsruhe, Germany.
<http://www.dgk-conference.de/>

27-31 March 2017

International Collaboration on Advanced Neutron Sources (ICANS XXII) Meeting, Oxford.
<http://icansxxii.iopconfs.org/home>

29 March – 11 April 2017

Expression, Purification & Analysis of Proteins and Protein Complexes, Cold Spring Harbor Laboratory, NY, USA.
<https://meetings.cshl.edu/courses.aspx?course=C-PPC&year=17>

29 March – 11 April 2017

Quantitative Imaging: From Cells to Molecules, Cold Spring Harbor Laboratory, NY, USA.
<https://meetings.cshl.edu/courses.aspx?course=C-QICM&year=17>

2-6 April 2017

253rd American Chemical Society National Meeting & Exposition, San Francisco, CA, USA.
https://www.acs.org/content/acs/en/meetings/spring-2017.html?cid=home_meetings

2-7 April 2017

OTST2017. Optical Terahertz Science and Technology, London.
<http://otst2017.iopconfs.org/home>

3-6 April 2017

DL_Software training workshop (3-5 April) followed by a Hack Day, London.
https://www CCP5.ac.uk/events/training_workshop.shtml

9-12 April 2017

Materiais 2017, Aveiro, Portugal.
<http://materiais2017.web.ua.pt/>

10-12 April 2017

40th Annual Meeting of the British Zeolite Association, Preston.
<http://www.bza.org/annual-meeting/>

10-12 April 2017

Chemical Physics of Electroactive Materials Faraday Discussion, Cambridge.
<http://www.rsc.org/events/detail/20368/chemical-physics-of-electroactive-materials-faraday-discussion>

10-13 April 2017

BCA Spring Meeting, Lancaster.
<http://www.bcaspringmeetings.org.uk/home>

10-13 April 2017

Interdisciplinary Surface Science Conference (ISSC-21), Manchester.
<http://issc21.iopconfs.org/home>

11-13 April 2017

Faraday Joint Interest Group Conference 2017, Warwick.
<http://www2.warwick.ac.uk/fac/sci/chemistry/news/events/faraday2017/>

17-21 April 2017

MRS Spring Meeting & Exhibit, Phoenix, AZ, USA.
<http://www.mrs.org/spring2017/>

18-21 April 2017

International Conference on Laser Energy Science / Laser and Accelerator Neutron Sources and Applications, Yokohama, Japan.
<http://lansa.opicon.jp/>

19-21 April 2017

Dielectrics, Teddington.
<http://dielectrics17.iopconfs.org/home>

22-26 April 2017

Hot topics in contemporary crystallography (HTCC), Poreč, Croatia.
<http://www.htcc2017.org/>

24-28 April 2017

INTERMAG Europe 2017. IEEE International Magnetics Conference, Dublin, Ireland.
<http://intermag2017.com/>

5-10 May 2017

Macromolecular Crystallography School 2017, Madrid, Spain.
<http://www.xtal.iqfr.csic.es/MCS2017/>

13-17 May 2017

Understanding Biology Through Structure 2017, Santa Fe, NM, USA.
https://conferences.newmexicoconsortium.org/conferences/ubts_17

14-17 May 2017

11th International Symposium on the Characterization of Porous Solids (COPS-XI), Avignon, France.
http://madirel.univ-amu.fr/web_pages_COPS/COPS_XI

14-18 May 2017

Protein quality control. Success and Failure in Health and Disease. Sant Feliu de Guixols, Spain.
<http://events.embo.org/17-quality-control/>

21-23 May 2017

EMBO/EMBL Symposium: Molecular and Cell Biology of Membranes, Heidelberg, Germany.
<http://www.embo-embl-symposia.org/symposia/2017/EES17-03/index.html>

22-26 May 2017

E-MRS Spring Meeting and Exhibit, Strasbourg, France.
<http://www.european-mrs.com/meetings/2017-spring-meeting>

25-26 May 2017

Instruct Biennial Structural Biology Meeting (IBSBM2017), Brno, Czech Republic.
<https://www.structuralbiology.eu/update/biennial2017>

26-30 May 2017

Annual Meeting of the American Crystallographic Association, New Orleans, LA, USA.
<http://www.amercrystalassn.org/content/pages/main-annual-meetings>

29 May – 2 June 2017

ISBC2017. 6th International School on Biological Crystallization, Granada, Spain.
<http://www.isbcgranada.org/>

29 May – 2 June 2017

Total Scattering for Nanotechnology on the Como Lake: To.Sca Lake 2.0, Como, Italy.
<http://tsnl.lakecomoschool.org/>

31 May – 3 June 2017

6th ALMA Conference 'painting as a Story' and 2nd CrysAC Workshop, Brno, Czech Republic.
<https://www.alma-lab.cz/eng/alma-conference-2017>

2-11 June 2017

International School of Crystallography 50th Course: Integrative Structural Biology, Erice (Sicily), Italy.
<https://crystalerice.org/2017/>

4-9 June 2017

IMMW20: International Magnetic Measurement Workshop, Diamond Light Source.
<http://www.diamond.ac.uk/Home/Events/2017/IMMW20.html>

5-7 June 2017

New directions in porous crystalline materials: Faraday Discussion, Edinburgh.
<http://www.rsc.org/events/detail/20413/new-directions-in-porous-crystalline-materials-faraday-discussion>

5-7 June 2017

canSAS: Small Angle Scattering Workshop, San Francisco, CA, USA.
<https://sites.google.com/a/lbl.gov/cansas/home>

5-9 June 2017

International Workshop on Computational Nanotechnology, Windermere.
<http://iwcn2017.iopconfs.org/home>

5-9 June 2017

8th Workshop on Neutron Scattering Applications in Structural Biology, Oak Ridge, TN, USA.
<https://conference.sns.gov/event/66/>

5-9 June 2017

Session I - Fundamentals of X-ray Powder Diffraction. ICDD X-ray Diffraction Clinic, Newtown Square, PA, USA.
<http://www.icdd.com/education/xrd.htm>

6-9 June 2017

4th NovAliX Conference: Biophysics in Drug Discovery 2017, Strasbourg, France.
http://www.idorganisation.com/v2/produits.php?langue=english&cle_menus=1238916384

7-9 June 2017

Neutrons in Structural Biology, Grenoble, France.
<https://indico.ill.fr/indico/event/58/>

11-22 June 2017

The Zurich School of Crystallography 2017: Bring Your Own Crystals, Zurich, Switzerland.
<http://www.chem.uzh.ch/linden/zsc/>

12-15 June 2017

Ultrafast X-ray Summer School (UXSS2017), Hamburg, Germany.
<https://conferences.cfel.de/uxss2017/>

12-16 June 2017

Session II - Advanced Methods in X-ray Powder Diffraction. ICDD X-ray Diffraction Clinic, Newtown Square, PA, USA.
<http://www.icdd.com/education/xrd.htm>

12-21 June 2017

Joint FEBS-EMBO Advanced Lecture Course: Molecular Architecture, Dynamics and Function of Biomembranes, Cargèse, Corsica, France.
<http://web.science.uu.nl/cargese2017/>

14-15 June 2017

Joint X-ray Diffraction and X-ray Fluorescence meeting, Leicester.
<http://www.crystallography.org.uk/>

19-23 June 2017

Mineral Fibres: Crystal Chemistry, Chemical-Physical Properties, Biological Interaction and Toxicity, Modena, Italy.
http://emu2017.unimore.it/wp-content/uploads/2016/03/EMU2017_flyer.pdf

19-26 June 2017

10th annual CCP4 crystallographic school "From data collection to structure refinement and beyond", Argonne, IL, USA.
<http://www ccp4.ac.uk/schools/APS-2017/index.php>

24-25 June 2017

Crystal Growth and Assembly (Gordon Research Seminar), Biddeford, ME, USA.
<http://www.grc.org/programs.aspx?id=17340>

25-30 June 2017

Gordon Research Conference on Crystal Growth and Assembly, Biddeford, ME, USA.
<http://www.grc.org/programs.aspx?id=12674>

26-30 June 2017

ICTMS 2017: 3rd International Conference on Tomography of Materials and Structures, Lund, Sweden.
<http://ictms2017.lth.se/>

27-29 June 2017

LCF8. Eighth International Conference on Low Cycle Fatigue, Dresden, Germany.
<http://www.lcf8.de/>

27-30 June 2017

48th BACG Annual Conference, Manchester.
<http://www.bacg-2017.co.uk/23786?platform=hootsuite>

27-30 June 2017

MLZ Conference Neutrons for Health, Bad Reichenhall, Germany.
<https://webapps.frm2.tum.de/indico/event/48/>

1-8 July 2017

4th Course of the Erice School: Neutron Science and Instrumentation, Erice, Sicily, Italy.
<http://sons.uniroma2.it/ericeneutronschool/iv-course/>

2-7 July 2017

4th European Crystallographic School (ECS4), Warsaw, Poland.
<http://ecs4.ecanews.org/>

3-5 July 2017

VHCF7. Seventh International Conference on Very High Cycle Fatigue, Dresden, Germany.
<http://www.vhcf7.de/>

3-6 July 2017

Microscience Microscopy Congress 2017, Manchester.
<http://www.mmc-series.org.uk/>

3-7 July 2017

7th FEZA Conference The ZEOLITES: Materials with Engineered Properties, Sofia, Bulgaria.
<http://feza2017.org/>

4 July 2017

Materials chemistry research and the economic health of the nation, Liverpool.
<https://www.liverpool.ac.uk/events/series/?seriesid=381>

6-14 July 2017

EMBO Practical Course: High-throughput protein production and crystallization, Harwell.
<http://meetings.embo.org/event/17-protein-production>

8-9 July 2017

FEZA School, Sofia, Bulgaria.
<http://feza2017.org/feza-school/>

9-13 July 2017

International Conference on Neutron Scattering 2017, Daejon, Republic of Korea.
<http://www.icns2017.org/>

10-12 July 2017

UK Colloids 2017, Manchester.
<http://constableandsmith.com/events/uk-colloids-2017>

10-13 July 2017

13th International Conference on Materials Chemistry (MC13), Liverpool.
<http://www.rsc.org/events/detail/21273/13th-international-conference-on-materials-chemistry-mc13>

16-20 July 2017

19th IUPAB Congress and 11th EBSA Congress, Edinburgh.
<http://www.iupab2017.org/home>

23-27 July 2017

16th European Conference on Solid State Chemistry, Glasgow.
<https://ecssc16.com/>

24-27 July 2017

PS31. Protein Society's 31st Annual Symposium, Montreal, Canada.
<http://www.proteinsociety.org/page/annual-symposium>

24-28 July 2017

9th International Conference on Borate Glasses, Crystals and Melts and 2nd International Conference on Phosphate Glasses, Oxford.

<http://www.borate-phosphate.sgt.org/>

30 July – 4 August 2017

21st American Conference on Crystal Growth and Epitaxy (ACCGE-21) and 18th US Workshop on Organometallic Vapor Phase Epitaxy (OMVPE-18), Santa Fe, NM, USA.
<http://www.crystalgrowth.org/Santa-Fe.html>

31 July – 4 August 2017

Denver X-ray Conference, Big Sky, MT, USA.
<http://www.dxcicdd.com>

6-10 August 2017

Microscopy & Microanalysis (M&M2017), St Louis, MO, USA.
<http://www.microscopy.org/MandM/2017/>

6-10 August 2017

X-ray Nanoimaging: Instruments and Methods III, San Diego, CA, USA.
<http://spie.org/OPO/conferencedetails/x-ray-nanoimaging>

14-15 August 2017

International Workshop on Improving Data Quality in XAFS Spectroscopy, Diamond Light Source.
<http://www.diamond.ac.uk/Home/Events/2017/Q2XAFS2017.html>

17-20 August 2017

Pharmaceutical Powder X-ray Diffraction Symposium, Hyderabad, India.
<http://www.icdd.com/pxrd/index.htm>

21-28 August 2017

24th Congress of the International Union of Crystallography, Hyderabad, India.
<http://www.iucr2017.org>

28 August – 1 September 2017

(IXS2017). 10th International Conference on Inelastic X-ray Scattering, DESY, Hamburg, Germany.
<https://indico.desy.de/conferenceDisplay.py?confId=13621>

30 August – 4 September 2017

International School on Fundamental Crystallography and Workshop on Structural Phase Transitions, Osisha, India.
<http://www.iucr2017.org/wp-content/uploads/2016/09/School.pdf>

3-6 September 2017

7th Cambridge Symposium on Nucleic Acids Chemistry and Biology, Cambridge.
<http://www.rsc.org/events/detail/23735/7th-cambridge-symposium-on-nucleic-acids-chemistry-and-biology>

3-8 September 2017

55th EHPRG Meeting: High Pressure Science and Technology, Poznan, Poland.
<http://www.ehprg2017.org/>

7-8 September 2017

Nanoanalysis and Structural Alloys, Drymen, Stirlingshire.
<http://nssa2017.iopconfs.org/home>

25-28 September 2017

WIRMS 2017- Infrared Microscopy and Spectroscopy with Accelerator Based Sources Workshop, Oxford.
<http://www.wirms2017.com/>

2-6 October 2017

Intermetallics Conference 2017, Bad Staffelstein, Germany.
<http://www.intermetallics-conference.de>

4-6 October 2017

6th Joint Workshop on High Pressure, Planetary and Plasma Physics (HP4), Göttingen, Germany.
<https://indico.desy.de/conferenceDisplay.py?confId=16402>

15-20 October 2017

6th Accelerator Reliability Workshop. ARW 2017, Versailles, France.
<http://www.synchrotron-soleil.fr/Workshops/2017/ARW-2017>

19-21 October 2017

The 75th Annual Pittsburgh Diffraction Conference, Indiana, PA, USA.
<http://www.pittdifsoc.org/conference.htm>

12-14 November 2017

25th Protein Structure Determination in Industry Meeting, Cambridge.
<http://www.psdi2017.org/25117>

26 November – 1 December 2017

2017 MRS Fall Meeting and Exhibit, Boston, MA, USA.
<https://www.mrs.org/fall2017>





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